

MATERIAL SAFETY DATA SHEET

National Institute of Standards and Technology
Standard Reference Materials Program
100 Bureau Drive, Stop 2320

Gaithersburg, Maryland 20899-2320

MSDS Coordinator: Mario Cellarosi
Telephone: 301-975-6776
FAX: 301-926-4751
E-mail: SRMMSDS@nist.gov

SRM Number: 3016
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SRM Name: *sec*-Butylbenzene
in Methanol

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Emergency Telephone ChemTrec:
1-800-424-9300 (North America)
+1-703-527-3887 (International)

SECTION I. MATERIAL IDENTIFICATION

Material Name: *sec*-Butylbenzene in Methanol

Description: SRM 3016 consists of two 5-milliliter sealed borosilicate glass ampoules, each containing approximately 2.5 mL of a solution of *sec*-butylbenzene in methanol.

Other Designations: *sec*-Butylbenzene (benzene, [1-methylpropyl]-;[1-methylpropyl] benzene; 2-phenylbutane; *sec*-butyl benzene; 2-phenyl butane; benzene, *sec*-butyl L; secondary-butyl benzene) in **Methanol** (methyl alcohol; wood alcohol; methyl hydroxide; carbinol; monohydroxymethane; wood spirit; wood naphtha; methylol)

Name	Chemical Formula	CAS Registry Number
Methanol	CH ₃ OH	67-56-1
<i>sec</i> -Butylbenzene	C ₆ H ₅ CH(CH ₃)C ₂ H ₅	135-98-8

DOT Classification: Methanol; UN1230; Packing Group II; Hazard Class 3.

SECTION II. HAZARDOUS INGREDIENTS

Hazardous Components	Nominal Concentration (%)	Exposure Limits and Toxicity Data
Methanol	99	OSHA TWA: 260 mg/m ³ (200 ppm)
		NIOSH recommended TWA (skin): 260 mg/m ³ (200 ppm) (10 h)
		NIOSH recommended STEL (skin): 325 mg/m ³ (250 ppm)
		UK WEL TWA (skin): 266 mg/m ³ (200 ppm)
		UK WEL STEL (skin): 333 mg/m ³ (250 ppm)
		Human, Inhalation TC _{LO} : 86 000 mg/m ³
		Human, Oral LD _{LO} : 143 mg/kg
		Man, Oral TD _{LO} : 3 429 mg/kg
<i>sec</i> -Butylbenzene	1	No occupational exposure limits established.
		Rat, Oral LD ₅₀ : 2 240 µL/kg
		Rat, Intermittent Oral TD _{LO} : 742 mg/kg (24 weeks)
		Rabbit, Skin LD ₅₀ : > 16 mL/kg

Carcinogenic, Tumorigenic, Mutagenic Reproductive Data: Methanol has been investigated as a mutagenic and reproductive effector.

SECTION III. PHYSICAL/CHEMICAL CHARACTERISTICS

Methanol	<i>sec</i>-Butylbenzene
Appearance and Odor: a clear, colorless liquid with a characteristic alcoholic odor	Appearance: a colorless liquid
Relative Molecular Mass: 32.04	Relative Molecular Mass: 134.22
Density: 0.7914 g/m ³	Density: 0.868 g/m ³
Boiling Point: 65 °C (149 °F)	Boiling Point: 173 °C (343 °F)
Freezing Point: -94 °C (-137 °F)	Freezing Point: -83 °C (-117 °F)
Vapor Pressure (@ 20 °C): 97.25 mmHg	Vapor Pressure (@ 60 °C): 15 mmHg
Evaporation Rate (butyl acetate = 1): 4.6	Evaporation Rate: not available
Viscosity (@ 20 °C): 0.59 cP	Viscosity: not available
Solubility in Water: soluble	Solubility in Water: insoluble
Solvent Solubility: soluble in ether, benzene, alcohol, acetone, chloroform, ethanol, ketones, and most organic solvents	Solvent Solubility: soluble in alcohol, benzene, acetone, and ether

NOTE: The physical and chemical data provided are for the pure components. Physical and chemical data for this methanol/*sec*-butylbenzene solution do not exist. The actual behavior of the solution may differ from the individual components.

SECTION IV. FIRE AND EXPLOSION HAZARD DATA

Methanol**Flash Point:** 11 °C**Method Used:** Closed Cup**Autoignition Temperature:** 385 °C**Flammability Limits in Air (Volume %):****UPPER:** 36**LOWER:** 6.0***sec*-Butylbenzene****Flash Point:** 52 °C**Method Used:** Closed Cup**Autoignition Temperature:** 418 °C**Flammability Limits in Air (Volume %):****UPPER:** 6.9**LOWER:** 0.8

Unusual Fire and Explosion Hazards: Methanol is a severe fire hazard. *sec*-Butylbenzene is a moderate fire hazard. Vapors are heavier than air and may travel a considerable distance to a source of ignition and flash back. Vapor and air mixtures are explosive above flash point.

Extinguishing Media: Use alcohol-resistant foam, regular dry chemical, carbon dioxide, or water spray.

Special Fire Procedures: Fire fighters should wear a self-contained breathing apparatus (SCBA) with a full face piece in the pressure demand or positive mode and other protective clothing.

SECTION V. REACTIVITY DATA

Stability: X **Stable** **Unstable**

Stable at normal temperatures and pressure.

Conditions to Avoid: Avoid contact with heat, sparks, flames, or other sources of ignition. Avoid inhalation of vapors or combustion by-products. Keep out of water supplies and sewers.

Incompatibility (Materials to Avoid): This material is incompatible with halo carbons, combustible materials, metals, oxidizing materials, halogens, metal carbide, amines, acids, and bases.

See Section IV: "Unusual Fire and Explosion Hazards".

Hazardous Decomposition or Byproducts: Thermal decomposition products may include toxic oxides of carbon and various organic fragments.

Hazardous Polymerization: **Will Occur** X **Will Not Occur**

SECTION VI. HEALTH HAZARD DATA

Route of Entry: X **Inhalation** X **Skin** X **Ingestion**

Methanol: Methanol is a skin and eye irritant and can cause nerve damage. This material is harmful if inhaled or absorbed through skin. Ingestion may be fatal or cause blindness. Symptoms of exposure may include burning sensation, coughing, wheezing, laryngitis, shortness of breath, headache, nausea, and vomiting. Exposure can cause damage to the eyes, liver, heart, and kidneys. Methanol may also cause gastrointestinal disturbances and convulsions.

sec-Butylbenzene: sec-Butylbenzene may cause mild to moderate irritation to skin, upper airway, mucous membranes, and eyes. This material is moderately toxic by ingestion.

Medical Conditions Generally Aggravated by Exposure: **Methanol** may cause eye disorders, kidney disorders, skin disorders, and allergies.

Target Organ(s) of Attack: Central nervous system (CNS).

Listed as a Carcinogen/Potential Carcinogen (Methanol):

	Yes	No
In the National Toxicology Program (NTP) Report on Carcinogens	<u> </u>	<u> X </u>
In the International Agency for Research on Cancer (IARC) Monographs	<u> </u>	<u> X </u>
By the Occupational Safety and Health Administration (OSHA)	<u> </u>	<u> X </u>

Listed as a Carcinogen/Potential Carcinogen (sec-Butylbenzene):

	Yes	No
In the National Toxicology Program (NTP) Report on Carcinogens	<u> </u>	<u> X </u>
In the International Agency for Research on Cancer (IARC) Monographs	<u> </u>	<u> X </u>
By the Occupational Safety and Health Administration (OSHA)	<u> </u>	<u> X </u>

EMERGENCY AND FIRST AID PROCEDURES:

Skin Contact: Remove contaminated shoes and clothing. Rinse affected area with large amounts of water followed by washing the area with soap and water. Watch for chemical irritations and treat them accordingly. Obtain medical assistance if necessary.

Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Obtain medical assistance.

Inhalation: If inhaled, move the victim to fresh air. If breathing is difficult, give oxygen; if the victim is not breathing, give artificial respiration by qualified personnel. Obtain medical assistance if necessary.

Ingestion: If ingested, obtain medical assistance immediately.

SECTION VII. PRECAUTIONS FOR SAFE HANDLING AND USE

Steps to be Taken in Case Material Is Released or Spilled: DO NOT touch spilled material. Reduce vapors with water spray. Avoid heat, flames, sparks, and other sources of ignition. Stop the leak if one can do so without risk. Absorb small spills with sand or other non-combustible absorbent material and place into containers for proper disposal.

Waste Disposal: Follow all federal, state, and local laws governing disposal. Methanol is subject to disposal regulations U.S. EPA 40 CFR 262, Hazardous Waste Number U154. *sec*-Butylbenzene is subject to disposal regulations U.S. EPA 40 CFR 262, Hazardous Waste Number D001.

Handling and Storage: Store and handle in accordance with all current regulations of standards. Keep methanol and *sec*-butylbenzene separated from incompatible substances. Persons handling this material must wear protective eyewear, clothing, and gloves to prevent contact with this material. Methanol and *sec*-butylbenzene are subject to storage regulations: U.S. OSHA 29 CFR 1910.106.

Sealed ampoules of SRM 3016 should be stored in the dark at temperatures between 10 °C and 30 °C. Protect containers from physical damage.

SECTION VIII. SOURCE DATA/OTHER COMMENTS

Sources: MDL Information Systems, Inc., MSDS *sec*-Butylbenzene, 16 June 2005.
MDL Information Systems, Inc., MSDS *Methyl Alcohol*, 16 June 2005.

Disclaimer: Physical and chemical data contained in this MSDS are provided only for use in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references; however, NIST does not certify the data on the MSDS. The certified value for this material is given in the NIST Certificate of Analysis.